OFFICE OF DEFENSE PROGRAMS

Summaries of materials activities which were selected to present the diversity of materials research, development and application projects conducted for the Office of the Assistant Secretary for Defense Programs are included in this section. Activities are organized in groupings that indicate the Defense Program Laboratory at which the specific project was performed. Funds for FY95 materials activities within Defense Programs were provided by the Weapons Research, Development and Test program including the Core Research and Development program and the Technology Transfer Initiative program and by the Inertial Confinement Fusion program, the Production and Surveillance program, and Laboratory Research and Development program. Projects with proprietary, patentable, or classified information were not reported.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

269. ENVIRONMENTALLY CONSCIOUS MANUFACTURING TECHNOLOGIES
$767,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project develops environmentally conscious manufacturing, ECM, technologies required for the manufacture of nuclear weapons components.

Keywords: Environmental

270. MICROELECTRONICS & PHOTONICS MATERIALS
$731,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project involves exploratory investigations into new semiconductor materials and heterostructures for photonic and microelectronic devices and systems. These investigations are expected to be foundational to the development of photonic and microelectronic technologies that will replace present day optical, electronic, electro-mechanical, and mechanical components and systems and offer more effective, efficient, compact, rugged, radiation hard, and electromagnetic pulse (EMP), resistant components for future generation systems.

Keywords: Semiconductors, Heterostructures

271. MICROMECHANICAL TECHNOLOGY
$1,822,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

Sandia presently has both an established surface micro mechanical technology and bulk micromechanical technology. Extensive internal and external customers exist for novel sensors and devices fabricated using these technologies. Most of these applications benefit from the integration of on-chip control and sense electronics, which lower costs, improve performance, decrease system size and increase manufacturability. These activities focus on the integration of Sandia's established digital/analog Complimentary Metal-Oxide Semiconductor (CMOS) technology with the existing micromechanical technologies.

Keywords: Micromechanical

272. CHEMICAL PROCESSING SCIENCE
$506,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project will advance the technology base that will enable: (1) intelligent design of chemical processes and reactors, (2) scientifically based optimization of processes and (3) in situ process monitors and sensors for real time control. We shall develop and maintain expertise in chemical vapor deposition (CVD) processes of importance to Microelectronics Development Laboratory (MDL) and Compound Semiconductor Research Laboratory (CSRL) in the fabrication of microelectronic and photonic devices. We shall develop and employ the scientific techniques of optical spectroscopies, chemical kinetics, surface science, and numerical modeling to address Si and III-V chemistry issues.

Keywords: Chemical Vapor Deposition, Modeling

273. **POLYMER SYNTHESIS, PROCESS & RELIABILITY**
$1,049,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The goal of this project is to expand our organic materials support capabilities through a science base in the following technology areas: (1) materials reliability and lifetime prediction; (2) optical and electronic materials, (3) molecular engineering of structural materials, (4) blends and interfaces, and (5) explosives aging.

Keywords: Polymers, Reliability

274. **POROUS & MICROPOROUS MATERIALS**
$1,439,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to develop a fundamental understanding of the synthesis, processing, characterization, and performance of porous and microporous materials for weapons and other applications. Specific applications include aging of polymeric materials for use in components such as neutron generators and explosively actuated power supplies, porous carbon electrode technology for use in rechargeable lithium batteries, and low dielectric polymers for electronics packaging.

Keywords: Polymers, Porous

275. **METAL JOINING TECHNOLOGIES**
$1,388,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project develops technologies required for the joining of metal hardware for Defense Programs. Specific applications include development of metal joining processes for environmentally conscious manufacturing and agile manufacturing. The subprojects encompass welding, soldering and brazing.

Keywords: Welding, Soldering, Brazing

276. **SMART PROCESSING OF MATERIALS**
$1,607,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The SMART processing project is formulated to provide synergy in the area of intelligent processing across a broad range of materials and processes. Research in this case is designed to dove-tail with the more applied SMART programs being supported under Defense Program (DP) capabilities. The products of the research are predictive scientific models or materials/processing knowledge which can be integrated or packaged for use in Model-based design systems. The funding for this project is divided among metals, ceramics, and polymers. In metals, three areas of process understanding are targeted: (1) characterization of the heat transfer process during welding; (2) microstructural evolution models for solidification of castings and welds; and (3) materials response models for predicting mechanical property/microstructural changes during large scale deformation processes such as forming/forging/welding. In the area of ceramics, the focus is in identifying the critical process parameters required to obtain homogenous properties in compacted ceramics as a function of particle size, shape, rheology and processing parameters. In the area of polymers, the focus is on developing the experimental data and process response maps needed to generate predictive models for mold filling and property evolution during curing or solidification of structural polymers.

Keywords: Processing, Welding, Powders, Polymers

277. **MATERIALS SCIENCE RESEARCH SUPPORT**
$276,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to provide program management support to research projects in the Engineered Materials & Processes portfolio at Sandia. One goal is to start new projects to meet strategic plan objectives, e.g., the electrochromic organic materials project, and SmartForge project.

Keywords: Forging, Electrochromic

278. **TEMPLATE-MEDIATED ONTOGENESIS: A NOVEL APPROACH TO MESOMORPHIC MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. E. Martin, (505) 844-9125

Mesomorphic materials have properties that are fundamentally different from those of their microscopic constituents. This frequently leads to greater utility, but producing mesoheterogeneous materials is often difficult since the only constraint imposed during synthesis is macroscopic-the reaction path itself. In this project, we use surfactant templates to produce novel mesoheterogeneous materials whose unique properties address specific materials goals. These include Chemically Selective

Filters, Size-Exclusion Chromatography Media; and an Optical Switch.

Keywords: Templates, Processing

279. **DYNAMICS OF NUCLEATION IN CHEMICAL VAPOR DEPOSITION**
$367,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

The structure and properties of a thin film are highly dependent on the conditions employed during growth. In particular, nucleation is known to be an important rate limiting step, and responsible for the evolution of the macroscopic structure for many materials. We have initiated a program to investigate nucleation in chemical vapor deposition of metals on silicon substrates for the purpose of understanding both the microscopic dynamics of growth processes and the relationship of these to the structure of the resulting film. We examine nucleation of Fe and Al on single crystal Si surfaces by thermal dissociation of suitable precursors in ultra high vacuum. We employ variable temperature scanning tunneling microscopy (STM) to directly image nucleation sites, structure of nuclei, and number and size distribution of nuclei in real time. These measurements will be complemented by global measures of structure, composition, and growth kinetics, including x-ray reflectivity (XRR), x-ray photoelectron spectroscopy (XPS), and reflection infrared spectroscopy (IR). We will also employ simulation and theoretical modeling of nucleation to test the sensitivity of structure to different dynamic processes and to examine the evolution of microstructure of the film.

Keywords: Nucleation, Chemical Vapor Deposition, Surfaces

280. **ATOMIC-SCALE MEASUREMENT OF LIQUID METAL WETTING AND FLOW**
$364,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

The wetting and flow of liquid metals plays an important role in materials synthesis and joining technologies. For example, soldering, brazing and welding require a liquid metal to wet the interface between two solids, and the fabrication of light-weight, metal-matrix structural composites involves the infiltration of a liquid metal into a porous ceramic preform. Despite the pervasive presence of liquid metal interfaces in materials problems, solutions are almost always the result of trial and error, rather than an atomic-scale scientific understanding. Just as microscopic flow processes determine the stability of atomically-thin grain boundary films, the wetting and flow of a macroscopic liquid are controlled by atomic motions at the leading edge of the spreading droplet. Current continuum models of spreading do not address atomic-scale flow mechanisms and fail to predict correctly wetting, flow, and stability of interfacial liquid metals. In this project we will (1) develop a new Acoustic Wave Damping experimental technique that can measure the atomic-scale flow behavior of liquid metals on solid substrates, and (2) use this technique to make the first viscoelastic measurements of well-characterized liquid metal layers. This project will have significant impact on scientific issues common to a wide variety of materials problems by providing new atomic level understanding that can be used to develop improved predictive engineering models for liquid flow and spreading phenomena.

Keywords: Wetting, Solder

281. **ATOMIC LAYER EPITAXIAL GROWTH OF DIAMOND USING HALOGENATED GASES**
$397,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: W. A. Hsu, (510) 294-2379

Atomic layer epitaxy (ALE) is a technique which has been exploited successfully in the area of compound semiconductors, such as the II-VI and III-V materials. The concept is to sequentially expose a substrate to alternating gaseous reagent species to build up, in an atomic layer-by-layer manner, the desired repeating compound layer structure. The reagent pairs that we are investigating in this technique include the CF_4/H_2 and CH_4/F_2 the systems. Our objectives are: (1) Deposit diamond at close to room temperature, (2) develop a process that is scalable to large area deposition, (3) control the deposition process so that it can potentially result in single crystal epitaxial growth.

Keywords: Diamond, Epitaxy

282. **DEVELOPMENT OF A SCALEABLE, FLAT-FLAME TECHNOLOGY FOR THE SYNTHESIS OF DIAMOND FILMS**
$384,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: K. F. McCarty, (510) 294-2067

We are developing a combustion technology that can be scaled to manufacture diamond films of arbitrary size. Flat-flames based on inherently scaleable stagnation flows give rapid and uniform diamond growth. A novel flow manifold, called a trumpet bell, is used to produce all the ideal properties of an infinite stagnation flow, but on a finite scale that maximizes the use of reagent gas. Computational modeling is used to understand and optimize the deposition process and to investigate potentially advantageous but high risk processes.

Keywords: Diamond, Processing

283. **SYNTHESIS AND PROCESSING OF HIGH STRENGTH SiC FOAMS: A RADICALLY NEW APPROACH TO CERAMIC-CERAMIC COMPOSITE MATERIALS**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. M. Hruby (510) 294-2596

Prohibitively high processing costs due to restricted fiber preform connectivity have kept silicon carbide, SiC, composites from entering mass commercial markets in spite of their favorable strength to weight ratio and oxidative stability. Our novel approach will bypass expensive fiber processing steps by providing a 3D interconnected network of struts having open connectivity to all pores. We propose several routes to synthesize and process the SiC foams. We will explore whether stressing the foams during pyrolysis can induce polymer chain alignment resulting in increased strength in the resulting SiC preform. This project will be the first sol gel entry into SiC materials, using designed precursor materials with the intent of preparing well defined foams. A variety of characterization techniques, including x-ray microtomography, x-ray diffraction, surface area, pore size distribution, and SEM, will be performed on the resulting new and unique materials. Many applications have been identified in an already large and growing area that would greatly benefit from near net shape processing, high strength, non-fiber processing, and energy savings.

Keywords: Ceramics, Porosity, SiC

284. **MOLECULAR ADHESION INCLUDING CHEMICAL REACTIONS AT POLYMER-SOLID INTERFACES**
$380,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: W. D. Wilson, (510) 294-2264

The goal of this project is to investigate mechanisms of adhesion of polymers to ionic, covalent, and metallic substrates. The program involves the development of a consistent model of surface atoms and polymeric functional groups which includes electrostatic, polarization and covalent effects. The embedded atom method of determining an atom's energy as a function of the total charge density at its center due to both molecules and solid atoms in its vicinity provides the underlying, unifying formalism.

Keywords: Adhesives, Polymers

285. **SYNTHESIS OF CERAMICS USING SUPERCRITICAL FLUIDS**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Adkins, (505) 845-9119

Supercritical fluids such as H_2O, CO_2, NH_3, etc., have unique solvation properties that make them appealing for the synthesis of materials that cannot be made by conventional means. If a solute-laden supercritical fluid is rapidly expanded through a nozzle, a powder is produced as the fluid expands. The rapid expansion of the fluid can lead to the production of unusual, nonequilibrium phases of the solute that might prove to be more readily sinterable. This technique combines the benefits of gas-phase powder synthesis with the high throughputs possible using spray technology. Waste minimization is automatic since the working fluid can be recycled. We will explore the use of supercritical fluids to synthesize novel (e.g., ultrafine, more reactive) ceramic powders.

Keywords: Supercritical, Powders

286. **CARBON NANOTUBE REINFORCED COMPOSITES**
$396,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. A. Cahill, (505) 844-5754

Carbon fiber composites are important advanced materials for applications from rocket casings to golf clubs because of their high strength to weight ratios. We propose to investigate carbon fiber composites in which the reinforcing carbon fibers are 1000 times smaller than the currently used micron-sized PAN or pitch derived fibers. This revolutionary decrease in the size of the fibers can be expected to lead to materials with greatly enhanced strength, stiffness, and durability. These improvements in physical properties are qualitatively predicted to be derived from: (1) the size of the fiber (because stress transfer from the matrix to the fiber becomes more efficient as the size of the fiber decreases and as the fiber surface area to weight ratio increases), and (2) the direct chemical reaction of the fiber with the matrix, which is generally not possible with micron sized carbon fibers, should lead to an extremely strong fiber-matrix interface. We propose to isolate pure 1-nanometer diameter carbon nanotubes from inexpensive, commercially-available, nanotube/soot mixtures, add solubilizing and reactive groups (as needed) to the side of the tubes, and fabricate fiber reinforced composite materials. Both the mechanical and dielectric (or conducting) properties of the composites will be fully characterized.

Keywords: Carbon, Composites

287. ADVANCED MATERIALS FOR BIOMEDICAL AND AEROSPACE APPLICATIONS
$217,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. T. McCord, (505) 844-5157

We have developed new materials and processes for hermetic glass-to-titanium seals that can be used in a variety of aerospace and biomedical electronic components. In particular, we have developed a new family of lanthanoborate sealing glasses that have the requisite thermal and chemical properties to form reliable seals. We have used these new glasses to produce prototype seals. We have characterized the interfacial reactions that lead to good chemical bonding between these glasses and titanium. We have also characterized biocompatible glasses in the Fe_2O_3- and TiO_2-CaO-P_2O_5 systems that also possess the thermal/chemical properties for titanium sealing.

Keywords: Glass, Seals, Biocompatible

288. CHEMICAL FUNCTIONAL OF OLIGOSILANES: ECONOMICALLY ATTRACTIVE ROUTES TO NEW PHOTORESPONSIVE MATERIALS
$393,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Renschler, (505) 844-0324

Polysilanes, [Si(R)(R')]n, are saturated macromolecules whose unusual electronic absorption behavior closely resembles those of conjugated polyenes. With synthetic routes previously available, they are not commercially viable as photointeractive materials, as current production (restricted to Japan) involves a very hazardous and unreliable synthetic approach. Low molecular weight oligosilanes can be formed under mild conditions, with reactive silane (Si-H) residues. We propose to utilize these oligo(hydrido)silanes as versatile precursors to a wide variety of new photoconductor materials with xerography and LED applications. Computer aided molecular design (CAMD) will be employed to select rational synthetic targets for oligosilane elaboration. Chemical modification at the Si-H bond will access numerous new oligosilanes and permit development of a wide variety of hybrid polymeric systems with novel polymer architectures; applications may include photoactive elastomers, thermoplastics and sensor materials, graft/block copolymers, LED display devices and controlled porosity thin films, fibers and monolithic bodies.

Keywords: Polymers, Displays, Photosensitive

289. POLYPHOSPHAACETYLENES: NEW CONDUCTING HYBRID ORGANIC-INORGANIC MATERIALS
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Renschler, (505) 844-0324

The purpose of this project has been to develop linear polyphosphaacetylenes, [P=C(R)]n, as a new class of conducting hybrid organic-inorganic polymer. Thermal, photochemical and transition metal-mediated metathesis polymerization of phosphaacetylene monomers are viewed as viable routes to the generation of formable polymeric materials with metal-like electrical conductivities. Expertise in computer aided molecular design has provided theoretical evidence that high electrical conductivities are achievable, as the organophosphorus polymeric backbones are predicted to be highly coplanar. Such materials should show conductivities superior to other conducting polymers reported to date. Synthetic efforts have established an efficient methodology to monomer fabrication, and design and synthesis of metathesis catalysts is underway.

Keywords: Polymer, Conductive, Synthesis

290. NEW ADHESIVE SYSTEMS BASED ON FUNCTIONALIZED BLOCK COPOLYMERS
$228,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

The need to control and optimize the properties of polymer/solid interfaces is critical in a host of technologies. Often the adhesive strength of the interface, the resistance to moisture, and the ability to transfer stress through the interface are critical to the overall performance of the product. A few specific examples include layers of conducting metals and polymer dielectrics in electronic packaging, filled rubber systems such as are used in the manufacture of tires, and structural adhesives. Recent evidence indicates that the adhesive failure in these interfaces often occurs a very short distance into the polymer matrix, typically 10-100 nm. This interphase region has proved difficult to design from first principles. Primer formulations involving small molecule coupling agents often must be tailored by a time consuming and inefficient trial and error process with very little underlying strategy. For many problems, adhesion is currently achieved by roughening surfaces in order to develop mechanical interlocking. This often involves the use of harsh chemicals which are hazardous to the environment. We propose to design and test new adhesive systems based on block copolymers, where one block (A) attaches to the surface while the second block (B) is compatible with and bonds to the polymeric matrix. An important advantage of block copolymers is that the B block can easily be made long enough to span the weak region of 10-100 nm and form a strong interlock with the matrix. We believe that these systems will lead to improved adhesion, more systematic design of the interphase region, and a decreased dependence on mechanical roughness and the environmentally unfriendly processes which are currently required.

Keywords: Adhesive, Polymer

291. **ENGINEERED MONODISPERSE POROUS MATERIALS**
$321,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

Porous materials are available with pore sizes ranging from 1's of Å to 100's of microns and beyond. Beyond 15Å it becomes difficult to obtain complete control over pore size, size-distribution, and ordering. We propose to use the novel properties of block copolymers to create monodisperse, controllable, ordered porous materials spanning the mesoporous range (20-500Å). Block copolymers consist of homopolymers chemically attached at their ends. These polymers want to phase separate from each other but are limited by the chemical attachment. The result is well-ordered, monodisperse, meso-size domains of one polymer surrounded by the other. We plan to make block copolymers where one phase can be crosslinked and the other phase can be chemically or thermally removed. This would give the desired controllable mesoporous materials. Block copolymer phase separation also gives a variety of architectures, including spherical, cylindrical, tetrahedral, and lamellar. These would lead to unique mesoporous architectures. In conjunction with the synthesis of these materials, we will be modeling our block copolymers using density functional theory, which can predict architecture based on the chemical and physical aspects of the block copolymer. This modeling will be useful in saving time and material. The synthetic technique we will use is called Ring Opening Metathesis Polymerization, and allows us to have tremendous control over polymer chain length, block ratios, and chemical composition. This control leads directly to control of the pore size and architecture. We will be analyzing our block copolymer materials to determine domain size, distribution, ordering, and architecture, both before and after pore formation. Both the modeling and synthesis of these well ordered, mesoporous, monodisperse materials is a novel approach to mesoporous material formation. These types of materials will have impact on several technology areas, including polymer separations, gas separations, remote sensor and bio-sensor materials, and catalyst supports.

Keywords: Polymer, Porous

292. **LOW-DIELECTRIC AND HIGH-TEMPERATURE FILMS FOR MULTICHIP MODULES**
$175,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

Thin low-dielectric and high-temperature films are used to separate multiple layers of patterned conductors in multichip module packaging. Significant improvements in processing speed could be obtained from the use of lower dielectric materials. We propose to obtain lower dielectric materials by preparing porous polymer films. Since the dielectric constant of air is close to that of vacuum, and much lower than any polymer, the porosity will lower the average dielectric constant of the film. To be able to prepare thin (<100 □m) films requires the use of very small-celled foams. We have substantial experience in this area, and have previously demonstrated the ability to prepare polymer films with cell sizes under 0.1 μm. In addition, porosities as high as 90 percent are attainable even with this small cell size. Conceivably, the dielectric constant of such a film will be reduced by as much as 90 percent of the difference between that of the bulk polymer and that of air. We propose to develop microcellular polyimide foams for this application. Polyimide is a high-temperature polymer used frequently for thin film dielectrics. In addition, we propose to develop the required processing techniques to allow us to concurrently prepare the foam and process it into its final form. This will involve the development of a process to spin-coat microcellular foams.

Keywords: Polymer, Dielectric, Thin Film

MATERIALS STRUCTURE AND COMPOSITION

293. **ADVANCED ANALYTICAL METHODS FOR MATERIALS RESEARCH**
$1,272,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project consists of several tasks, each of which is a relatively independent analytical methods development activity including: advanced microanalysis development; chemometrics; surface polymer contamination characterization; by x-ray diffraction in thin films; metal impurity characterization on semiconductor surfaces; sensor development and x-ray and ion beam tomography.

Keywords: Analysis, Diffraction, Tomography

294. **ADAPTIVE SCANNING PROBE MICROSCOPIES**
$417,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

In the short time that Scanning Probe Microscopies (SPM) have been on the scene, they have demonstrated great potential to contribute to fundamental materials science problems, process science studies and new approaches to production quality control. However, the simple data acquisition and analysis procedures that are currently used severely restrict our ability to extract quantitative information regarding, for example, atomic scale rate processes or local chemical compositions. In this project we will develop a new paradigm for operating SPMs whereby the microscope adapts its data acquisition to focus on the most important features of the structure under examination. Currently, SPMs scan a region of material by devoting an equal amount of time to all areas of the image. However, for most materials problems, only the data that are associated with specific features such as defects or possibly nucleation centers are used to analyze the state of the material. An adaptive scanning approach could be used to locate, track and image features of interest without the overhead of acquiring data over the entire sample region. By using this approach, the time required to collect information will be decreased by several orders of magnitude, which will enable us to study kinetic processes with unprecedented microscopic-real-space resolution. In addition, current SPMs do not make use of the range of electronic data they can locally generate, so that chemical information on an atomic scale is usually not acquired. Pattern recognition techniques will be applied to these local data to distinguish and recognize features based on local electronic properties of the surface. The ability of the instrument to recognize specific features will greatly increase the operators ability to examine and analyze complex materials structures. This new capability will place us in a strong position to apply SPMs to a wider range of technologically important problems such as catalysis, corrosion, lubrication and biological processes.

Keywords: Scanning Probe Microscopy, Surfaces

295. **CHARACTERIZATION AND CORRELATION OF PHYSICAL PROPERTIES OF CERAMICS THROUGH ORIENTATION IMAGING MICROSCOPY**
$122,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. F. Green, (505) 845-8929

This program is intended to be the proof-of-principle of an innovative approach to characterizing polycrystalline materials through orientation imaging microscopy. We propose to explore the use of the backscattered electron Kikuchi pattern (BEKP) technique for performing orientation imaging microscopy. This technique provides the crystallographic misorientation between adjoining grains, which should allow us to develop a more complete understanding of the relationship between grain boundary structure and properties, and the overall properties of a polycrystalline body. We are specifically interested in the relationship between the crystallographic misorientation and the fracture behavior of materials; however, crystallographic misorientation data are potentially as important for other properties and behavior.

Keywords: Microscopy, Microstructure

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

296. **ENERGETIC MATERIAL CENTER**
$106,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. J. Allen, (505) 845-9624

This project provides funds to perform collaborative program formulations with Lawrence Livermore National Laboratory in energetic materials, high explosives, pyrotechnics, and rocket fuels to fulfill the common mission goals of Science Based Stockpile Stewardship and Product Realization.

Keywords: Energetic Materials

297. **COMPUTATIONAL SOLID DYNAMICS**
$2,716,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: E. H. Barsis, (505) 845-8938

The purpose of this project is to develop and validate computational models for the response of materials to a spectrum of dynamic and quasi-static loading conditions that are required in the design of nuclear components and systems.

Keywords: Models, Stress

298. **APPLIED MATERIALS & MECHANICS COLLABORATIONS**
$635,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project supports thirty-one separate projects in which Sandia staff collaborate with graduate students. Projects include work on low flux/low residue solders, development of hard tribological materials for stronglink application, sensor development, modeling of materials response in mixed environments, development of corrosion-resistant glasses for hermetic seals, modeling of composite materials, and development of advanced polymeric materials.

Keywords: Solders, Tribological, Corrosion

299. **DEVELOPMENT OF MORE EFFICIENT POWER SOURCES**
$1,044,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Mangan, (505) 845-9538

The purpose of this project is to: (1) develop a state-of-the-art carbon anode for lithium ion rechargeable batteries and demonstrate its performance by building a prototype that demonstrates performance and manufacturability; (2) develop materials, device design and a working prototype of an advanced double layer capacitor; and (3) evaluate self-discharge kinetics to permit precise lifetime projections for Lithium/Titanium Carbide, Li/TC, Batteries. The project involves collaboration with domestic Lithium/Titanium Carbide producers to transfer our fundamental understanding of this system, enabling them to enter the growing market for high reliability, long life Lithium/Titanium Carbide batteries.

Keywords: Batteries, Carbon, Reliability

300. **BASIC SCIENCE OF MATERIALS STABILITY**
$1,829,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. L. Mattern, (505) 845-9490

The purpose of this project is to: (1) develop and apply atomic- and molecular-level microscopies, spectroscopies, and theoretical models in order to examine fundamental materials processes that control phenomena including: interfacial adhesion, lubrication, wear, thermal stability, thin-film and surface kinetics, radiation effects, corrosion, hydrogen effects, curing, fracture, and chemical and physical vapor deposition processes; (2) develop scientific basis for design, manufacture and application of small smart products; (3) transfer degradation resistant/stable materials technology to DOE defense program applications and to U.S. advanced materials industries and develop new models for predicting useful lifetimes for currently used materials and structure.

Keywords: Surfaces, Microscopy

301. **ADVANCED MATERIALS CHARACTERIZATION SCIENCE**
$1,006,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. L. Mattern, (505) 845-9490

The purpose of this project is to: (1) maintain, utilize and develop new state-of-the-art materials analysis/characterization techniques of general applicability to microelectronics photonics, materials research, energy, advanced testing, and weapons programs; (2) develop new approaches to test, quantify and understand/predict the performance of materials/components used in advanced weapon systems under normal or extreme conditions; (3) develop ultra-high resolution accelerator microbeam methods and utilize for submicron radiation exposure /imaging of integrated circuits (ICs) and components to be used in radiation environments (e.g., space, fission/fusion reactors, nuclear battlefield, etc.); (4) invent/perfect advanced atomic-level in situ and ex situ diagnostics based on x-ray diffraction and atom-force microscopy; (5) initiate new programs utilizing advanced characterization techniques and/or transfer technology to other Defense Program (DP) lab/industry; (6) publish/patent new techniques and communicate results to Defense Program.

Keywords: Microbeams, Radiation, Diffraction

302. **PHOTONICS TECHNOLOGY**
$1,206,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project establishes exploratory investigations into new concepts for photonic structures, devices, and systems. These investigations are foundational to the development of photonic technologies that will replace present day optical, electronic, electro-mechanical, and mechanical components and systems and will offer more effective, efficient, compact, rugged, radiation hard, and electromagnetic (EMP) resistant components.

Keywords: Photonics

303. **ELECTRONIC CERAMICS**
$899,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to advance the chemistry and physics basis for the fabrication and use of electrically and optically active ceramics. One goal of this project is to investigate the basic chemistry of sol-gel processes in order to develop an intelligent and versatile approach to thin-film fabrication. Specific goals are to: (1) develop processing methods for producing optimized microstructures for ferroelectric thin films; (2) determine microstructures that enhance or suppress 90 degree domain switching in ferroelectric films; (3) investigate effects of thin-film stresses and microstructure on piezoelectric activity; (4) determine the relative contributions of various cations to ferro-electricity in perovskites; (5) determine defects that lead to intrinsic luminescence in zinc oxide phosphors; (6) investigate dopants to enhance red, green and blue luminescence in zinc oxide; (7) investigate degradation mechanisms in perovskite thin films.

Keywords: Ceramics, Ferroelectric, Piezoelectric

304. **ULTRAHARD MATERIALS RESEARCH**
$594,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to develop and enhance research capabilities in the synthesis, characterization, and materials development that relate to nitrides, carbides, diamond, and diamond-like carbon. Specific tasks include: (1) investigate the mechanisms of film growth; (2) characterize the mechanical, electrical, and atomic structure of these materials; and (3) explore weapons and dual-use applications for these materials.

Keywords: Nitrides, Diamond

305. **IMPURITY EFFECTS ON INTERFACES**
$997,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The major objective of this project is to quantify the permeation and trapping of impurities in metals, alloys, and inorganic materials and to relate these phenomena to embrittlement of grain boundaries, bi-crystals, coatings, and engineering materials. Theoretical models are developed to describe adhesion of metal films on ceramic oxide surfaces.

Keywords: Interfaces, Reliability, Films

306. **MATERIALS AGING & RELIABILITY**
$1,155,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project provides significant advances in the science-based stockpile stewardship of non-nuclear components by combining the interdisciplinary capabilities of materials science, high performance computing, integrated sensors, and advanced engineering simulation. The focus of the project is to advance the understanding of microstructural mechanisms which control the reliability and performance of materials. This understanding is translated into a mathematical description to allow improved predictive capabilities based on the development/deployment of integrated sensors and/or advanced simulations. An important goal is to support materials science work that is combined into projects that draw support and leverage from research. The combination of material (mathematical) modeling, and high performance computing and advanced engineering simulation transfers materials understanding into practical predictor tools that can be applied to the stockpile, as well as to commercial products and applications. Specific sensor development can then be based on the fundamental understanding of the materials behavior of the sensor as well as the signature of the specific event/degradation being sensed.

Keywords: Prediction, Models, Reliability

307. **ENGINEERING SCIENCES RESEARCH**
$6,157,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. J. Hommert, (505) 844-3449

The project is divided into four main elements that constitute the work areas within engineering sciences. These elements are Computational Methods for Engineering Analysis, Material Mechanics, Experimental Mechanics, and Manufacturing and Material Processes. Under each of these main program elements there are specific research tasks that are intended to further the engineering science capabilities available to apply to the laboratories applications. Specific projects include: (1) develop computational methods and models of energetic materials to predict multiphase effects; (2) develop new techniques for the prediction of lifecycle reliability using material response models for the prediction of aging and fatigue; (3) develop new models of polymer response for analysis of curing and shrinkage of seals and other components to enable improved design; (4) develop new material response models that bridge microscopic to macroscopic descriptions; (5) develop and apply experimental methods to validate advanced material response models; (6) implement advanced material response characterization into models of welding, stamping, material removal and coatings for advanced manufacturing processes; (7) improve the capability for finite element analysis of large deformations and material non-linearities through contact algorithms, shell elements and adaptivity; (8) develop gridless solver technology for application to component design and performance analysis; (9) develop the capability to implement non-deterministic and optimization simulation concepts in finite element analysis; (10) develop advanced fluid mechanics capabilities for the description of turbulent eddies for describing fire propation; (11) develop the capability to predict the response of cellular foams and distended materials for crash applications; and (12) develop models of energetic materials for predicting deflagration to detonation.

Keywords: Models, Mechanics, Processing

308. **GAS SEPARATION OF FULLERENE MEMBRANES**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. E. Schirber, (505) 844-8134

Industrially important gas separation processes such as the removal of nitrogen from natural gas and separation of nitrogen and oxygen consume enormous amounts of energy. Most membrane separation processes are based on amorphous polymeric films which contain a broad distribution of pore sizes through which gas molecules diffuse at different rates. We have discovered that the lattice of fullerene C_{60} can function as a permeation barrier. Since the diffusion pathway is precisely defined by the channels between interstitial sites, we expect that the lattice will exhibit large separation factors for appropriate gas pairs and that the permeation rate can be made very high for thin films. In this study we propose to characterize the permeation process, model the separation process, prepare membranes by the sublimation of thin fullerene films on suitable substrates, measure the resulting separation factors and permeation rates, and address engineering aspects of preparing a functional membrane system.

Keywords: Separation, Membrane, Fullerene

309. **PbO-FREE COMPOSITES FOR LOW TEMPERATURE PACKAGING**
$359,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. F. Green, (505) 845-8929

We will develop a new class of inorganic materials that will have the requisite thermal and chemical properties to replace PbO-solder glasses currently used in a variety of low temperature packaging applications. These new materials will be composites of low temperature, chemically stable glasses and low expansion, chemically compatible ceramics. Composites will be designed with thermal contraction coefficients between 70 and 100 x 10^{-7}/°C and seal temperatures below 450°C so that they can replace PbO-solder glasses used to seal flat panel displays, alumina sensor packages, and other hermetic packages.

Keywords: Solder, Lead-free, Packaging

310. **DEMONSTRATION OF MOLECULAR-BASED TRANSISTORS**
$317,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: R. F. Clough, (505) 844-3492

Photonics and electronics technologies continue toward miniaturization, but these technologies are based largely on main-group semiconductors. An alternative approach lies in using macromolecular building blocks to build very small circuits. Research in the area of conducting polymers represents one of the first forays of chemists into this arena. A crucial element in any logic circuit is a transistor, in which a base current regulates the current between collector and emitter. We propose to develop optically-gated organic transistors based on photochromic organic conducting polymers. The operation of such a device would parallel that of a normal transistor, but the current switching would depend on both the electronic and structural changes in the polymer induced by photo-reactions instead of a base current. Such a device represents a new method for integration of electronic and photonic processing. Intensive research on conducting polymers has narrowed the field of candidates viable for device applications. Polythiophene is an environmentally stable conducting polymer for which very high conductivities have been reported. In addition, many different routes are available to synthesize the required monomers and polymers. These features combine to make polythiophene an excellent candidate for device applications, and thus polythiophene derivatives will be the initial focus of our efforts. A photochromic compound is one that isomerizes from an initial form A to a different form B when irradiated with light of wavelength 1, and B in turn isomerizes to A when irradiated with light of wavelength 2. The conformational and electronic differences between such photoisomers will provide the mechanism for switching conductivity on and off in the proposed polymers. The overall goals of this project are (1) to provide examples of photoswitched conductivity in organic molecules and (2) to use this ability to fabricate microscale photoswitches and demonstrate their use in binary arrays (memory devices).

Keywords: Polymers, Transistors, Molecular

311. **NANOCOMPOSITE MATERIALS BASED ON HYDROCARBON-BRIDGED SILOXANES**
$442,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Ulibarri, (505) 844-5279

Silicones [polydimethylsiloxane (PDMS) polymers] are environmentally safe, nonflammable, weather resistant, thermally stable, low Tg materials that are attractive for general elastomer applications because of their safety and performance over a wide temperature range. However, PDMS is inherently weak due to its low glass transition temperature (Tg) and lack of stress crystallization. Fortunately, reinforced materials with suitable properties can be generated by mechanically blending PDMS polymers with pyrogenic silicas. While the U.S. is still the major producer of silicones, foreign competitors are gaining market share due to their improved technology and product quality as they duplicate and modify U.S. technology. Since silicone elastomers are used in numerous military and civilian applications, it is critical that significantly new manufacturing technologies be developed in the U.S. Recent work has indicated that two other ways to enhance elastomer strength are the use of bimodal polymer distributions and the introduction of hydrocarbon fragments into the polymer matrix. However, the origin of the improved properties cannot be fully understood and investigated in the systems presently available. We have devised a method which, for the first time, will allow us to completely control the length and identity of the short chain molecule and the hydrocarbon linkage. PDMS-based composite materials containing a variety of alkylene-and arylene-bridged polysilsesquioxanes will be synthesized in order to probe short chain and linkage effects in bimodal polymer networks. Monte Carlo simulations will be performed as a function of chain length to predict the optimal chain lengths required for maximum reinforcement. PRISM calculations will be performed on the PDMS/silsesquioxane blends as a function of molecular weight in order to understand the phase separation characteristics of the system. The silsesquioxane-PDMS networks will be synthesized and evaluated both as unfilled materials and as sol-gel generated silica-filled materials. Analysis of the mechanical properties of the materials will be coupled with molecular and structural analysis in order to determine structure/property relationships.

Keywords: Composite, Polymer

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

312. **MC4300 NEUTRON TUBE**
$329,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. J. Bohrer, (510) 294-3111

This project provides funds to design and develop in a timely and cost effective manner, a universal neutron tube satisfying the requirements of all stockpile weapons by the year 2002; specifically to evolve a design which minimizes fabrication parts and processing through studies to advance technologies such as diffusion bonding, ion optics, and cermets.

Keywords: Processing, Joining, Cermets

313. **SMARTWELD II**
$1,985,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project continues the development of SMARTWELD. SMARTWELD is a concurrent engineering system which integrates product design and processing decisions within an electronic desktop engineering environment. It is being developed to provide the designer with transparent access to people, information, tools and past experience. Empirical understanding, along with process models, are synthesized within a knowledge-based system to identify the most optimal fabrication procedures based on cost, schedule, performance or environmental impact. Integration of the process simulation tools with design tools will enable the designer to assess a number of design and process options on the computer rather than on the manufacturing floor. Task models and generic process models are being embedded within user friendly Graphics User Interfaces, GUIs, to more readily enable the customer to use the SMARTWELD system without extensive training. The integrated system architecture under development will provide interactive communications and shared application capabilities across a variety of workstation and PC-type platforms either locally or at remote sites.

Keywords: Welding, Models

314. **MANUFACTURING TECHNOLOGY**
$1,859,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project consists of three major efforts: (1) IMPReS which includes the integrated modeling and processing of resin-based structures and the extension of the SmartWeld paradigm 12 to polymer-based materials and structures; and (2) Advanced Process Controllers, which includes the development of controller hardware for brilliant real-time model-based control of manufacturing processes; and (3) Assembly Scripting which involves development of automatic assembly planning and scripting algorithms and systems.

Keywords: Polymers

315. **ELECTRONIC AND MICROELECTROMECHANICAL SYSTEMS (MEMS) COMPONENTS**
$1,416,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: W. R. Reynolds, (505) 844-3087

This project provides funds to: (1) develop stronglinks in several steps starting with use of micromachining technology to develop parts, then integrate parts to make stonglink; (2) develop all-quartz and integrated silicon-quartz resonators for small clocks and sensors for DOE, military and commercial applications; and (3) develop and characterize low temperature weaklink capacitor and coil and develop/characterize fiber optic sensors.

Keywords: Micromachining, Capacitors, Sensors

INSTRUMENTATION AND FACILITIES

316. **MATERIALS PROCESSES FOR MANUFACTURING**
$703,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project will consist of two areas to enhance manufacturing capabilities: Virtual Reality and Development Plating Facility. *Virtual Reality* - This project will build on recent developments at Sandia. Free-form rapid prototyping, robotics, on-machine inspection coupled with sophisticated solid models and process models are rapidly emerging areas that will be evaluated and improved. *Development Plating Facility* - Finalize design and complete construction of new Development Plating Facility in the Advanced Manufacturing Process Center (AMPL).

Keywords: Prototyping, Models, Plating

LAWRENCE LIVERMORE NATIONAL LABORATORY

317. **ENGINEERED NANOSTRUCTURE LAMINATES**
$1,800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (510) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500□m thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection x-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

318. **SOL GEL COATINGS**
$335,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: I. M. Thomas, (510) 423-4430 and J. Britten, (510) 423-7653

We continue to investigate the preparation of multilayer sol-gel high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2. We have found that the incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection.

A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is to be delivered in early FY 1994.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings